Dr. Michael George Lerner   lernerm@nhlbi.nih.gov   (301) 451-2014

EDUCATIONAL AND PROFESSIONAL EXPERIENCE

NIH/NHLBI   **Rockville, MD**
IRTA Postdoctoral Fellow   Dec. 2007 - Present
Research Advisor: Dr. Richard Pastor

University of Michigan   **Ann Arbor, MI**
Ph.D.: Biophysics   Jan. 2004 - Nov. 2007
Advisor: Prof. Heather A. Carlson
Dissertation: "Computational studies of *E. coli* DHFR: Drug design, dynamics and method development."
M.S.: Biophysics Research Division   Aug. 2001 - Dec. 2003

Ricoh Silicon Valley   **Cupertino, CA**
Software Engineer   1999 - 2001
- Design and implementation of both UI and low-level components
- Language design and implementation.
- Professional experience with C++, Python, C, SSML, HTML, JavaScript and Perl.

Haverford College   **Haverford, PA**
B.S.: Physics   May 1999
Concentration: Computer Science
Advisor: Prof. Walter Smith
Honors: Departmental Honors in Physics
Thesis Title "Some Applications of Scanning Tunneling Microscopy to the Study of Proteins."

RESEARCH EXPERIENCE

Laboratory of Computational Biology, NIH/NHLBI   **Rockville, MD**
Postdoctoral Researcher with Dr. Richard Pastor and Dr. Bernard Brooks   Dec. 2007 – Present
- Simulation and analysis of coarse-grained lipid bilayers
  - Examined differences between all-atom and coarse-grained simulations
  - Discovered system-size dependence of physical parameters (lateral diffusion constants)
  - Modeled diffusion of tethered proteins and tethered lipids in DPPC bilayers
  - Investigated effects of hydration on NMR order parameters
  - Development of multi-scale models for simulations of lipid bilayers
- Quasiharmonic vibrational subsystem analysis
  - Development and implementation of novel techniques

Biophysics Research Division, University of Michigan   **Ann Arbor, MI**
Graduate Research Assistant with Prof. Heather A. Carlson   May 2002 - Nov. 2007
- Developed and refined of multiple protein structure (MPS) methods for incorporating protein flexibility into structure-based drug design.
  - Developed a novel method for placing small chemical probes into active sites.
  - Developed a new Jarvis-Patrick based method for clustering small chemical probes.
  - Verified MPS method via application to protein-protein binding interfaces.
  - Automated and sped up the MPS method and applied it to dihydrofolate reductase (DHFR) to discover general and species-specific novel inhibitors.
- Investigating dynamics and catalysis of DHFR via molecular dynamics.
  - Discovered transient patterns of correlated dynamics in DHFR•NADPH complex.
  - Discovered potential new allosteric site.
- Collaborated to create a non-redundant database of protein-ligand complexes in order to study the basic biophysics of protein-ligand interaction.

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Biophysics Research Division, University of Michigan   **Ann Arbor, MI**
Graduate Research Assistant with Prof. Nils Walter   Dec. 2001 - May 2002
- Studied the hairpin ribozyme using Fluorescence Resonance Energy Transfer (FRET).

Biophysics Research Division, University of Michigan   **Ann Arbor, MI**
Graduate Research Assistant with Prof. Samuel Krimm   Aug. 2001 - Dec. 2001
- Parameterized of methanol for a spectroscopically determined force field.

Physics Department, Haverford College   **Haverford, PA**
Physics Research Assistant with Prof. Walter Smith   May 1998 - May 1999
- Used scanning tunneling microscopy (STM) to study proteins and self-assembled monolayers.
- Designed and created self-assembling monolayers to adhere streptavidin to a gold (111) substrate.
- Discovered a novel and useful method of nanolithography.
- Undergraduate thesis title: "**Some Applications of Scanning Tunneling Microscopy to the Study of Proteins**."

Mathematics Department, Haverford College   **Haverford, PA**
Mathematics Research Assistant with Prof. Stephanie Singer   May 1997 - July 1997
- Studied symplectic geometry at the Park City Mathematics Institute, administered by the Institute for Advanced Studies.
- Investigated economic applications of Noether's Theorem, applying variational principles to search for conservation laws in economic systems.

Astronomy Department, Haverford College   **Haverford, PA**
Astronomy Research Assistant with Prof. Stephen Boughn   May 1996 - July 1996
- Studied the possibility of using the earth as a detector of gravitational waves.

PUBLICATIONS
- **Lerner, M. G.**; Kravitz, J. Y.; Carlson, H. A., The PyMOL-APBS plugin: A tool for automated electrostatics calculations and computational Alanine scanning, *manuscript in preparation*.
- **Lerner, M. G.**; Carlson, H. A., Correlated and conformational dynamics of the DHFR•NADPH complex, *manuscript in preparation*.
- **Lerner, M. G.**; Spronk, S. A.; Carlson, H. A., PyPAT: A Python-based toolset to aid in the analysis of protein structures and trajectories, *manuscript in preparation*.
- **Lerner, M. G.**; Meagher, K. L.; Carlson, H. A., Automated clustering of probe molecules from solvent mapping of protein surfaces, *J. Comput. Aided Mol. Des. 2008, 10, 727-736*.
- **Lerner, M. G**.; Bowman, A. L.; Carlson, H. A., Incorporating Dynamics in E. coli Dihydrofolate Reductase Enhances Structure-based Drug Discovery*, J. Chem. Inf. Model. 2007, 47, 2358-2365*.
- Bowman, A. L.; **Lerner, M. G.**; Carlson, H. A., Protein flexibility and species specificity in structure-based drug discovery: Dihydrofolate reductase as a test system. *J. Am. Chem. Soc.* 2007, 129 (12), 3634-3640.
- Meagher, K. L.; **Lerner, M. G.**, Carlson, H. A., Refining the multiple protein structure method: consistency across three independent HIV-1 protease models. *J. Med. Chem.* 2006, 49, (12), 3478-3484.
- Hu, L.; Benson, M. L.; Smith, R. D.; **Lerner, M. G.**; Carlson, H. A., Binding MOAD (Mother of All Databases). *Prot. Struct. Func. Bioinformatics* 2005, 60, 333-340.

OPEN SOURCE SOFTWARE DEVELOPED

- PyMOL-APBS Plugin. Integrates the PyMOL molecular graphics system with APBS to enable rapid, easy calculation of electrostatic potential surfaces with minimal user intervention. Included with recent versions of PyMOL.

CONFERENCES, WORKSHOPS AND PRESENTATIONS

- Conference: American Chemical Society Fall 2009 national meeting, August 2009
- National Institutes of Health NHLBI DIR Fellows Retreat, March 2009.
  - Poster presenter and author: A comparison of translational and rotational dynamics of coarse-grained and all-atom lipid bilayers. Lerner, M. G.; Lee, H., Pastor, R. W.
- National Institutes of Health NHLBI DIR Fellows Retreat, March 2008.
  - Poster presenter and author: Dihydrofolate reductase: Computational investigations of dynamics and drug design. Lerner, M. G.; Carlson, H. A.; Brooks B. R.
- Conference: Biophysical Society annual meeting, February 2008.
- Conference: 229th National ACS Meeting, San Diego, CA, March 2005.
  - Poster presenter and author: Automatic Clustering of Probe Molecules to Define Surface Complementarity: Applications to Protein-Protein Interfaces. Lerner, M. G.; Carlson, H. A.
  - Poster author: Binding MOAD (Mother of All Databases). Benson, M. L.; Hu, L.; Smith, R. D.; Lerner, M. G.; Carlson, H. A.
  - Poster author: Incorporating Protein Flexibility into Drug Design: HIV-1 Protease as a Test Case. Meagher, K. L.; Lerner, M. G.; Carlson, H. A.
- Conference: Modeling Protein Flexibility and Motions, Banff International Research Station, July 2004.
- Seminar: Molecular Biophysics Training Grant Seminar, University of Michigan, 2003-2006.
  - Oral presentation: Binding MOAD (Mother of All Databases): Developing a Non-redundant Dataset. 2003.
  - Oral presentation: Dihydrofolate Reductase as a Test System for Computational Drug Discovery. 2004.
  - Oral presentation: Refining the MPS Method: Flooding and Clustering. 2005.
  - Oral presentation: Applying the MPS Method to DHFR for Structure-based Drug Design. 2006.
- Poster: Molecular Biophysics Symposium, University of Michigan, 2003-2006, given yearly on current research.
- Conference: Symplectic Geometry, Park City Mathematics Institute, Park City, Utah, 1997. Hosted by the Institute for Advanced Studies.

TECHNICAL SKILLS

- *Software Applications*: CHARMM, GROMACS, AMBER, PyMOL, MOE, OpenEye (OMEGA), BOSS (MUSIC), APBS, VMD, Chimera, ChemOffice, CAVER.
- *Computing Environments*: Unix, Linux, OS X and Windows.
- *Programming Languages*: Professional experience in Python and C++, significant experience with C, SSML, HTML, JavaScript and Perl, some experience with FORTRAN.
- *Technical Writing and Reviewing*: Experience writing and reviewing manuscripts for publication in peer-reviewed journals.

TEACHING EXPERIENCE

Department of Medicinal Chemistry, University of Michigan   **Ann Arbor, MI**
Mentor   May 2006 - Present

- Supervised an undergraduate student for a Research Experience for Undergraduates (REU) summer program (research on this project is ongoing).
- Mentored student in computational chemistry and molecular modeling.

- Taught hands-on implementation of the scientific method, specifically hypothesis development and testing with computer simulations.

Physics Department, University of Michigan   **Ann Arbor, MI**
Graduate Student Instructor   Sept. 2006 - Dec. 2006
- Taught calculus-based electricity and magnetism labs for four sections (approximately 100 students) of physics and engineering students. These are standalone labs, with no required concurrent lecture.
- Received **Outstanding Graduate Student Instructor** award, given to the best first-time graduate student instructor in the physics department (based on student and faculty evaluations).

Center for Research on Learning and Teaching, University of Michigan   **Ann Arbor, MI**
Michigan Teaching Fellow   Summer 2006
- Attended summer-long seminar and training series designed to prepare a select group of advanced graduate students for faculty positions by developing teaching and professional skills.
- Learned about aspects of the higher education system, including differences in culture and expectations among types of colleges and universities, the nature of today's students and other forces affecting faculty work.
- Read literature about and discussed a number of pedagogical topics, e.g. multicultural teaching, instructional technology and current research on teaching and learning.
- Prepared a statement of teaching philosophy, a teaching portfolio and a syllabus.

Ricoh Silicon Valley   **Cupertino, CA**
- Trained new employees in the use of CVS, SSML, Python and other tasks. 1999 - 2001

City Year   **Chicago, IL**
Corps Member   1996-1997
- Tutored and mentored fourth and fifth graders at Brian Piccolo Elementary School as part of a full time, yearlong community service program for 17-24 year olds.
- Designed and presented several fourth and fifth grade science lessons.
- Patient care at Casa Central, a community-based nursing home.

Mathematics Department, Haverford College   **Haverford, PA**
Mathematics Question Center   1994 - 1999
- Tutored undergraduate students in Calculus (single- and multi-variable), Differential Equations, Abstract Algebra, Real Analysis, Statistics, Discrete Mathematics and other courses for four years.

FELLOWSHIPS AND HONORS
- IRTA Postdoctoral Fellow (NIH/NHLBI)   Dec. 2007 - Present
- Outstanding Graduate Instructor (University of Michigan Physics Dept.)   2007
- Michigan Teaching Fellow (University of Michigan)   2006
- Molecular Biophysics Training Grant (NIH)   May 2003 - Apr. 2005
- Undergraduate Research Fellowship from the Council on   Sept. 1997 - Apr. 1999
  Undergraduate Research (CUR)

PROFESSIONAL ORGANIZATIONS
- American Chemical Society
- American Association for the Advancement of Science
- American Association of Physics Teachers
- Biophysical Society